Posterior Covariance vs. Analysis Error Covariance in Data Assimilation

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Overview

- Introduction
- Analysis Error Covariance via Hessian
- Posterior Covariance : A Bayesian approach
- Effective Covariance Estimates
- Implementation : some remarks
- Asymptotic Properties
- Numerical Example
- Conclusion

Introduction 1

There are two basic approaches for Data Assimilation:

- Variational Methods
- Kalman Filter

Both lead to minimize a cost function :

$$J(u) = \frac{1}{2}(V_b^{-1}(u - u_b), u - u_b)_X + \frac{1}{2}(V_o^{-1}(C\varphi - y), C\varphi - y)_{Y_o}, \quad (1)$$

where $u_b \in X$ is a prior initial-value function (background state), $y \in Y_o$ is a prescribed function (observational data), Y_o is an observation space, $C : Y \to Y_o$ is a linear bounded operator.
We get the same optimal solution $\bar{u}$

Introduction 2

$\bar{u}$ is the solution of the Optimality System :

$$\left\{ \begin{array}{rcl} \dfrac{\partial \varphi}{\partial t} & = & F(\varphi) + f, \quad t \in (0, T) \\ \varphi\Big|_{t=0} & = & u, \end{array} \right. \tag{2}$$

$$\left\{ \begin{array}{rcl} \dfrac{\partial \varphi^*}{\partial t} + (F'(\varphi))^* \varphi^* & = & C^* V_o^{-1}(C\varphi - y), \quad t \in (0, T) \\ \varphi^*\Big|_{t=T} & = & 0, \end{array} \right. \tag{3}$$

$$V_b^{-1}(u - u_b) - \varphi^*\Big|_{t=0} = 0 \tag{4}$$

Introduction 3

In an analysis there are two inputs:

- The background u_b
- the observation y

Both have error and the question is what is the impact of these errors on the analysis?

The background can be considered from two different viewpoints:

- Variational viewpoint: the background is a regularization term in the Tykhonov's sense to make the problem well posed
- Bayesian view point: the background is an a priori information on the analysis

Introduction 4

In the linear case we get the same covariance error for the analysis : the **inverse of the Hessian** of the cost function.

In the non linear case we get two different items:

- Variational approach : Analysis Error Covariance
- Bayesian Approach : Posterior Covariance

Questions:

- How to compute, approximate, these elements?
- What are the differences?

Analysis Error Covariance 1: True solution and Errors

We assume the existence of a "true" solution u^t and an associated "true" state φ^t verifying:

$$\left\{ \begin{array}{rcl} \frac{\partial \varphi^t}{\partial t} & = & F(\varphi^t) + f, \quad t \in (0, T) \\ \varphi^t\big|_{t=0} & = & u^t. \end{array} \right. \tag{5}$$

Then the errors are defined by : $u_b = u^t + \xi_b,\ y = C\varphi^t + \xi_o$ with covariances V_b and V_o

Analysis Error Covariance 2: Discrepancy Evolution

Let

$$\delta\varphi = \varphi - \varphi^t, \ \delta u = u - u^t.$$

Then for regular F there exists $\tilde{\varphi} = \varphi^t + \tau(\varphi - \varphi^t), \ \tau \in [0,1]$, such that

$$\left\{ \begin{array}{rcl} \frac{\partial \delta\varphi}{\partial t} - F'(\tilde{\varphi})\delta\varphi & = & 0, \quad t \in (0,T), \\ \delta\varphi\big|_{t=0} & = & \delta u, \end{array} \right. \tag{6}$$

$$\left\{ \begin{array}{rcl} \frac{\partial \varphi^*}{\partial t} + (F'(\varphi))^*\varphi^* & = & C^* V_o^{-1}(C\delta\varphi - \xi_o), \\ \varphi^*\big|_{t=T} & = & 0, \end{array} \right. \tag{7}$$

$$V_b^{-1}(\delta u - \xi_b) - \varphi^*|_{t=0} = 0. \tag{8}$$

Analysis Error Covariance 3: Exact Equation for Analysis Error

Let us introduce the operator $R(\varphi) : X \to Y$ as follows:

$$R(\varphi)v = \psi, \; v \in X, \tag{9}$$

where ψ is the solution of the tangent linear problem

$$\frac{\partial \psi}{\partial t} - F'(\varphi)\psi = 0, \; \psi|_{t=0} = v. \tag{10}$$

Then, the system for errors can be represented as a single operator equation for δu:

$$H(\varphi, \tilde{\varphi})\delta u = V_b^{-1}\xi_b + R^*(\varphi)C^*V_o^{-1}\xi_o, \tag{11}$$

where

$$H(\varphi, \tilde{\varphi}) = V_b^{-1} + R^*(\varphi)C^*V_o^{-1}CR(\tilde{\varphi}). \tag{12}$$

Analysis Error Covariance 4 : H Operator

The operator $H(\varphi,\tilde{\varphi}) : X \to X$ can be defined by

$$\frac{\partial \psi}{\partial t} - F'(\tilde{\varphi})\psi = 0,\ \psi|_{t=0} = v, \tag{13}$$

$$-\frac{\partial \psi^*}{\partial t} - (F'(\varphi))^*\psi^* = -C^* V_o^{-1} C\psi,\ \ \psi^*\Big|_{t=T} = 0, \tag{14}$$

$$H(\varphi,\tilde{\varphi})v = V_b^{-1} v - \psi^*|_{t=0}. \tag{15}$$

The operator $H(\varphi,\tilde{\varphi})$ is neither symmetric, nor positive definite. $\varphi = \tilde{\varphi} = \theta$, it becomes the Hessian $H(\theta)$ of the cost function J_1 in the following auxiliary DA problem: find δu and $\delta\varphi$ such that $J_1(\delta u) = \inf\limits_{v} J_1(v)$, where

$$J_1(\delta u) = \frac{1}{2}(V_b^{-1}(\delta u - \xi_b), \delta u - \xi_b)_X + \frac{1}{2}(V_o^{-1}(C\delta\varphi - \xi_o), C\delta\varphi - \xi_o)_{Y_o}, \tag{16}$$

and $\delta\varphi$ satisfies the problem

$$\frac{\partial \delta\varphi}{\partial t} - F'(\theta)\delta\varphi = 0,\ \delta\varphi\Big|_{t=0} = \delta u. \tag{17}$$

Analysis Error Covariance 5 : Analysis Error Covariance via Hessian

The optimal solution (analysis) error δu is assumed to be unbiased, i.e. $E[\delta u] = 0$, and

$$V_{\delta u} \cdot = E[(\cdot, \delta u)_X \; \delta u] = E[(\cdot, u - u^t)_X \; (u - u^t)]. \tag{18}$$

The best value of φ and $\tilde{\varphi}$ independent of ξ_o, ξ_b is apparently φ^t and using

$$R(\tilde{\varphi}) \approx R(\varphi^t), \; R^*(\varphi) \approx R^*(\varphi^t), \tag{19}$$

the error equation reduces to

$$H(\varphi^t)\delta u = V_b^{-1}\xi_b + R^*(\varphi^t)C^* V_o^{-1}\xi_o, \quad H(\cdot) = V_b^{-1} + R^*(\cdot)C^* V_o^{-1} CR(\cdot). \tag{20}$$

We express δu from equation (**??**)

$$\delta u = H^{-1}(\varphi^t)(V_b^{-1}\xi_b + R^*(\varphi^t)C^* V_o^{-1}\xi_o)$$

and obtain for the **analysis error covariance**

$$V_{\delta u} = H^{-1}(\varphi^t)(V_b^{-1} + R^*(\varphi^t)C^* V_o^{-1} CR(\varphi^t))H^{-1}(\varphi^t) = H^{-1}(\varphi^t). \tag{21}$$

Analysis Error Covariance 6 : Approximations

In practice the 'true' field φ^t is not known, thus we have to use an approximation $\bar{\varphi}$ associated to a certain optimal solution $\bar{u}$ defined by the real data $(\bar{u}_b, \bar{y})$, i.e. we use

$$V_{\delta u} = H^{-1}(\bar{\varphi}). \tag{22}$$

In (Rabier and Courtier,1992), the error equation is derived in the form

$$(V_b^{-1} + R^*(\varphi)C^* V_o^{-1} CR(\varphi))\delta u = V_b^{-1}\xi_b + R^*(\varphi)C^* V_o^{-1}\xi_o. \tag{23}$$

The error due to transitions $R(\tilde{\varphi}) \to R(\varphi^t)$ and $R^*(\varphi) \to R^*(\varphi^t)$; we call it the 'linearization' error. The use of $\bar{\varphi}$ instead of φ^t in the Hessian computations leads to another error, which shall be called the 'origin' error.

Posterior Covariance : Bayesian Approach 1

Given $u_b \sim \mathcal{N}(\bar{u}_b, V_b)$, $y \sim \mathcal{N}(\bar{y}, V_o)$, the following expression for the posterior distribution of u is derived from the Bayes theorem:

$$p(u|\bar{y}) = C \cdot \exp\left(-\frac{1}{2}(V_b^{-1}(u-\bar{u}_b), u-\bar{u}_b)_X\right) \cdot \exp\left(-\frac{1}{2}(V_o^{-1}(C\varphi-\bar{y}), C\varphi-\bar{y})_{Y_o}\right). \tag{24}$$

The solution to the variational DA problem with the data $y = \bar{y}$ and $u_b = \bar{u}$ is equal to the mode of $p(u, \bar{y})$ (see e.g. Lorenc, 1986; Tarantola, 1987). Accordingly, the Bayesian posterior covariance is defined by :

$$\mathcal{V}_{\delta u} \cdot = E[(\cdot, u - E[u])_X \, (u - E[u])] \tag{25}$$

with $u \sim p(u|\bar{y})$.

Posterior Covariance : Bayesian Approach 2

In order to compute $\mathcal{V}_{\delta u}$ by the Monte Carlo method, one must generate a sample of pseudo-random realizations u_i from $p(u|\bar{y})$. We will consider u_i to be the solutions to the DA problem with the perturbed data $u_b = \bar{u}_b + \xi_b$, and $y = \bar{y} + \xi_o$, where $\xi_b \sim \mathcal{N}(0, V_b)$, $\xi_o \sim \mathcal{N}(0, V_o)$. Further we assume that $E[u] = \bar{u}$, where $\bar{u}$ is the solution to the unperturbed problem in which case $\mathcal{V}_{\delta u}$ can be approximated as follows

$$\mathcal{V}_{\delta u} \cdot = E[(\cdot, u - \bar{u})_X \, (u - \bar{u})] = E[(\cdot, \delta u)_X \, \delta u]. \tag{26}$$

Posterior Covariance : O.S. for Errors

Unperturbed O.S. with $u_b = \bar{u}_b$, $y = \bar{y}$:

$$\frac{\partial \bar{\varphi}}{\partial t} = F(\bar{\varphi}) + f,\ \varphi\Big|_{t=0} = \bar{u}, \tag{27}$$

$$\frac{\partial \bar{\varphi}^*}{\partial t} + (F'(\bar{\varphi}))^* \bar{\varphi}^* = C^* V_o^{-1}(C\bar{\varphi} - \bar{y}),\ \ \bar{\varphi}^*\Big|_{t=T} = 0, \tag{28}$$

$$V_b^{-1}(\bar{u} - \bar{u}_b) - \bar{\varphi}^*\Big|_{t=0} = 0 \tag{29}$$

With perturbations : $u_b = \bar{u}_b + \xi_b$, $y = \bar{y} + \xi_o$, where $\xi_b \in X, \xi_o \in Y_o$.
$\delta u = u - \bar{u}$, $\delta\varphi = \varphi - \bar{\varphi}$, $\delta\varphi^* = \varphi^* - \bar{\varphi}^*$.

$$\frac{\partial \delta\varphi}{\partial t} = F(\varphi) - F(\bar{\varphi}),\ \delta\varphi\Big|_{t=0} = \delta u, \tag{30}$$

$$\frac{\partial \delta\varphi^*}{\partial t} + (F'(\varphi))^* \delta\varphi^* = [((F'(\bar{\varphi}))^* - F'(\varphi))^*]\bar{\varphi}^* + C^* V_o^{-1}(C\delta\varphi - \xi_o), \tag{31}$$

$$V_b^{-1}(\delta u - \xi_b) - \delta\varphi^*\Big|_{t=0} = 0. \tag{32}$$

Posterior Covariance : Exact Errors Equations

Introducing $\tilde{\varphi}_1 = \bar{\varphi} + \tau_1 \delta\varphi$, $\tilde{\varphi}_2 = \bar{\varphi} + \tau_2 \delta\varphi$, $\tau_1, \tau_2 \in [0,1]$, we derive the exact system for errors:

$$\frac{\partial \delta\varphi}{\partial t} = F'(\tilde{\varphi}_1)\delta\varphi, \ \delta\varphi\big|_{t=0} = \delta u, \tag{33}$$

$$\frac{\partial \delta\varphi^*}{\partial t} + (F'(\varphi))^* \delta\varphi^* = [(F'(\tilde{\varphi}_2))^* \bar{\varphi}^*]' \delta\varphi + C^* V_o^{-1}(C\delta\varphi - \xi_o), \tag{34}$$

$$V_b^{-1}(\delta u - \xi_b) - \delta\varphi^*\big|_{t=0} = 0, \tag{35}$$

equivalent to a single operator equation for δu:

$$\mathcal{H}(\varphi, \tilde{\varphi}_1, \tilde{\varphi}_2)\delta u = V_b^{-1}\xi_b + R^*(\varphi) C^* V_o^{-1} \xi_o, \tag{36}$$

where

$$\mathcal{H}(\varphi, \tilde{\varphi}_1, \tilde{\varphi}_2) = V_b^{-1} + R^*(\varphi)(C^* V_o^{-1} C - [(F'(\tilde{\varphi}_2))^* \bar{\varphi}^*]') R(\tilde{\varphi}_1). \tag{37}$$

Posterior Covariance : Operator $\mathcal{H}$

$\mathcal{H}(\varphi, \tilde{\varphi}_1, \tilde{\varphi}_2) : X \to X$ is defined by solving:

$$\frac{\partial \psi}{\partial t} = F'(\tilde{\varphi}_1)\psi, \; \psi\Big|_{t=0} = v, \tag{38}$$

$$-\frac{\partial \psi^*}{\partial t} - (F'(\varphi))^*\psi^* = [(F'(\tilde{\varphi}_2))^*\bar{\varphi}^*]'\psi - C^* V_o^{-1} C\psi, \tag{39}$$

$$\mathcal{H}(\varphi, \tilde{\varphi}_1, \tilde{\varphi}_2)v = V_b^{-1} v - \psi^*\Big|_{t=0}. \tag{40}$$

If we had $\varphi = \tilde{\varphi}_1 = \tilde{\varphi}_2$, $\mathcal{H}(\varphi)$ becomes the Hessian of the cost function in the original DA problem, it is symmetric and positive definite if u is a minimum of $J(u)$. The equation is often referred as the 'second order' adjoint (Le Dimet et al., 2002).

As above, we assume that $E(\delta u) \approx 0$, and we consider the following approximations

$$R(\tilde{\varphi}_1) \approx R(\bar{\varphi}), \;\; R^*(\varphi) \approx R^*(\bar{\varphi}), \;\; [(F'(\tilde{\varphi}_2))^*\bar{\varphi}^*]' \approx [(F'(\bar{\varphi}))^*\bar{\varphi}^*]'. \tag{41}$$

Posterior Covariance via Hessian

The exact error equation (**??**) is approximated as follows

$$\mathcal{H}(\bar{\varphi})\delta u = V_b^{-1}\xi_b + R(\bar{\varphi})^* C^* V_o^{-1}\xi_o, \tag{42}$$

where

$$\mathcal{H}(\cdot) = V_b^{-1} + R^*(\cdot)(C^* V_o^{-1} C - [(F'(\cdot))^* \bar{\varphi}^*]')R(\cdot). \tag{43}$$

Now, we express δu :

$$\delta u = \mathcal{H}^{-1}(\bar{\varphi})(V_b^{-1}\xi_b + R(\bar{\varphi})^* C^* V_o^{-1}\xi_o),$$

and obtain an approximate expression for the **posterior error covariance**

$$\mathcal{V}_1 = \mathcal{H}^{-1}(\bar{\varphi})(V_b^{-1} + R^*(\bar{\varphi})V_o^{-1}R(\bar{\varphi}))\mathcal{H}^{-1}(\bar{\varphi}) = \mathcal{H}^{-1}(\bar{\varphi})H(\bar{\varphi})\mathcal{H}^{-1}(\bar{\varphi}), \tag{44}$$

where $H(\bar{\varphi})$ is the Hessian of the cost function J_1 computed at $\theta = \bar{\varphi}$.
Other approximations of the posterior covariance:

$$\mathcal{V}_2 = \mathcal{H}^{-1}(\bar{\varphi}), \;\; \mathcal{V}_3 = H^{-1}(\bar{\varphi}). \tag{45}$$

Posterior Covariance : "Effective" Estimates

To supress the linearization errors, the 'effective' inverse Hessian may be used for estimating the analysis error covariance (see Gejadze et al., 2011):

$$V_{\delta u} = E\left[H^{-1}(\varphi)\right]. \tag{46}$$

The same is true for the posterior error covariance $\mathcal{V}_{\delta u}$:

$$\mathcal{V}_{\delta u} = E\left[\mathcal{H}^{-1}(\varphi,\tilde{\varphi}_1,\tilde{\varphi}_2)\; H(\varphi)\; \mathcal{H}^{-1}(\varphi,\tilde{\varphi}_1,\tilde{\varphi}_2)\right].$$

First, we substitute a possibly asymmetric and indefinite operator $\mathcal{H}(\varphi,\tilde{\varphi}_1,\tilde{\varphi}_2)$ by $\mathcal{H}(\varphi)$:

$$\mathcal{V}_{\delta u} \approx \mathcal{V}_1^e = E\left[\mathcal{H}^{-1}(\varphi)\; H(\varphi)\; \mathcal{H}^{-1}(\varphi)\right]. \tag{47}$$

Next, by assuming $H(\varphi)\mathcal{H}^{-1}(\varphi) \approx I$ we get

$$\mathcal{V}_{\delta u} \approx \mathcal{V}_2^e = E\left[\mathcal{H}^{-1}(\varphi)\right]. \tag{48}$$

Finally, by assuming $\mathcal{H}^{-1}(\varphi) \approx H^{-1}(\varphi)$ we obtain yet another approximation

$$\mathcal{V}_{\delta u} \approx \mathcal{V}_3^e = E\left[H^{-1}(\varphi)\right]. \tag{49}$$

Numerical Example

$\varphi(x,t)$ is governed by the 1D Burgers equation with a nonlinear viscous term :

$$\frac{\partial \varphi}{\partial t} + \frac{1}{2}\frac{\partial(\varphi^2)}{\partial x} = \frac{\partial}{\partial x}\left(\nu(\varphi)\frac{\partial \varphi}{\partial x}\right), \tag{50}$$

$$\varphi = \varphi(x,t),\ t \in (0,T),\ x \in (0,1),$$

with the Neumann boundary conditions

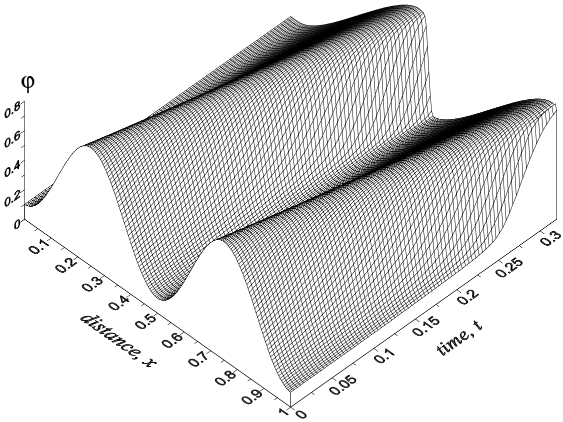
$$\left.\frac{\partial \varphi}{\partial x}\right|_{x=0} = \left.\frac{\partial \varphi}{\partial x}\right|_{x=1} = 0 \tag{51}$$

and the viscosity coefficient

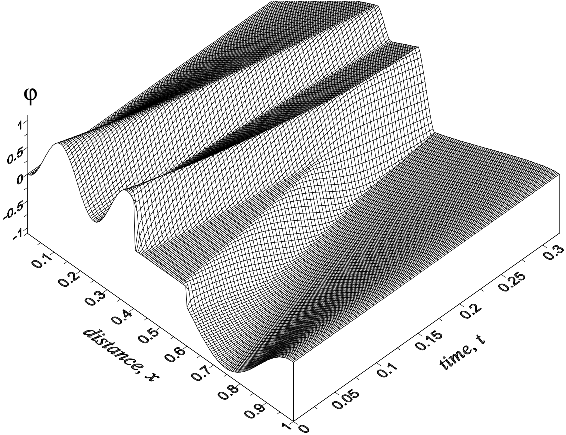
$$\nu(\varphi) = \nu_0 + \nu_1\left(\frac{\partial \varphi}{\partial x}\right)^2,\ \ \nu_0, \nu_1 = const > 0. \tag{52}$$

Two initial conditions $u^t = \varphi^t(x,0)$ are considered (case A and case B),

Numerical Example : Cas A



Numerical Example : Cas B

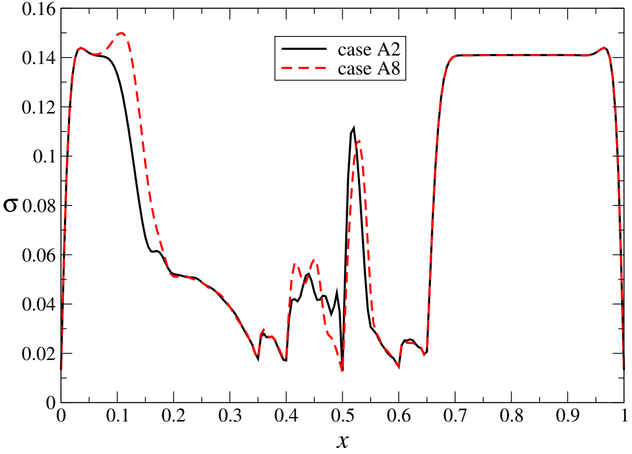


Numerical Example : Squared Riemann distance

$$\mu(A,B) = \left(\sum_{i=1}^{M} ln^2\gamma_i\right)^{1/2}.$$

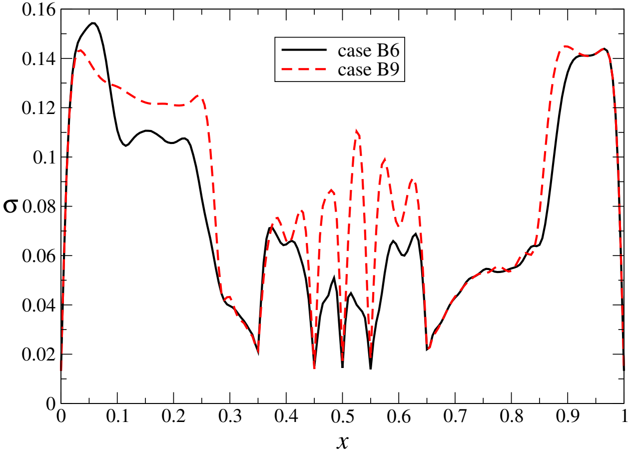
Case	$\mu^2(\mathcal{V}_3,\hat{\mathcal{V}})$	$\mu^2(\mathcal{V}_2,\hat{\mathcal{V}})$	$\mu^2(\mathcal{V}_1,\hat{\mathcal{V}})$	$\mu^2(\mathcal{V}_3^e,\hat{\mathcal{V}})$	$\mu^2(\mathcal{V}_2^e,\hat{\mathcal{V}})$	$\mu^2(\mathcal{V}_1^e,\hat{\mathcal{V}})$
$A1$	3.817	3.058	4.738	2.250	1.418	1.151
$A2$	17.89	18.06	21.50	2.535	1.778	1.602
$A5$	5.832	5.070	5.778	3.710	2.886	2.564
$A7$	20.21	19.76	22.24	4.290	3.508	3.383
$A8$	1.133	0.585	1.419	1.108	0.466	0.246
$A9$	20.18	20.65	24.52	2.191	1.986	1.976
$A10$	10.01	8.521	8.411	3.200	2.437	2.428
$B1$	7.271	6.452	6.785	2.852	1.835	1.476
$B2$	16.42	14.89	14.70	15.61	14.11	13.77
$B3$	9.937	10.70	17.70	4.125	3.636	3.385
$B4$	6.223	5.353	11.50	2.600	1.773	1.580
$B5$	10.73	9.515	9.875	4.752	3.178	2.530
$B6$	6.184	4.153	8.621	4.874	2.479	1.858

The reference mean deviation $\hat{\sigma}(x)$ (related to $\hat{\mathcal{V}}$). Cases A2, A8.

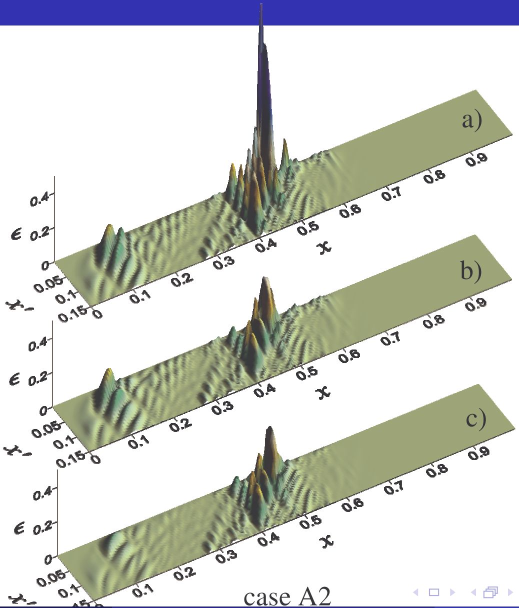


The mean deviation vector σ is defined as follows: $\sigma(i) = \mathcal{V}^{1/2}(i, i)$.

The reference mean deviation $\hat{\sigma}(x)$ (related to $\hat{\mathcal{V}}$). Cases B6, B9.

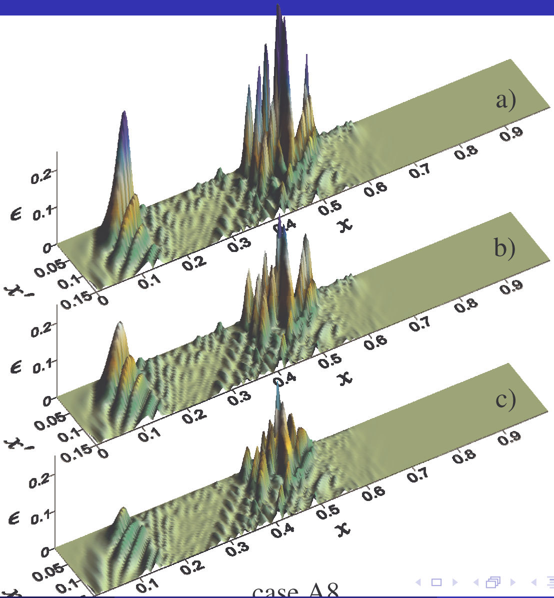


Absolute errors in the correlation matrix: ϵ_3, ϵ_3^e, ϵ_1^e (case A2)

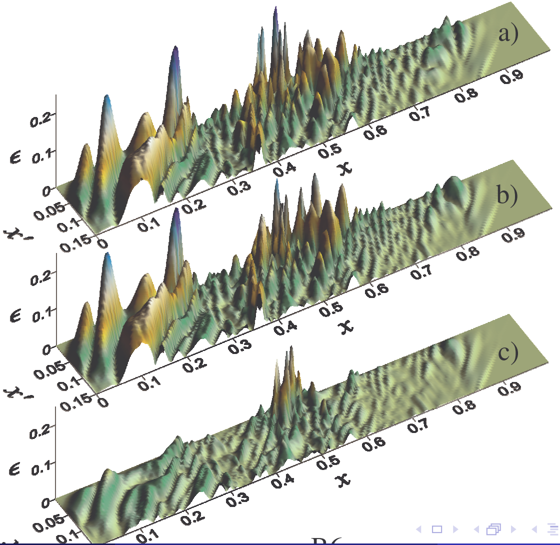


case A2

Absolute errors in the correlation matrix: ϵ_3, ϵ_3^e, ϵ_1^e (case A8)



Absolute errors in the correlation matrix: ϵ_3, ϵ_3^e, ϵ_1^e (case B6)



Conclusion

- Variational and Bayesian approaches of DA lead to the minimization of the same function
- For Error Estimation we obtain two different concepts
  - Analysis Error Covariance for the Variational Approach
  - Posterior Covariance for the Bayesian Approach
- In the linear case the covariances coincide
- In the nonlinear case strong discrepancies can occur.
- Algorithms for the estimation and the approximation of these covariances are proposed.

Gejadze, I.,Shutyaev, V., Le Dimet, F.-X. **Analysis error covariance versus posterior covariance in variational data assimilation problems. Q.J.R.Meteolol. Soc. (2013).**